

Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(43) 11927–12388 (2023)



Cover
See Dario Neri, Nicholas Favalli *et al.*, pp. 12026–12033. Image reproduced by permission of Sara Puglioli and Nicholas Favalli on behalf of Philochem AG from *Chem. Sci.*, 2023, 14, 12026.



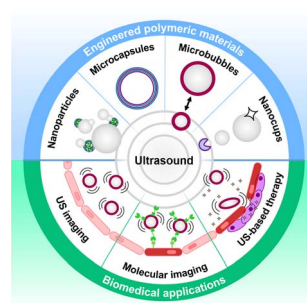
Inside cover
See Mark Gandelman *et al.*, pp. 12034–12040. Image reproduced by permission of Idan Avigdor from *Chem. Sci.*, 2023, 14, 12034.

PERSPECTIVE

11941

Polymeric materials for ultrasound imaging and therapy

Roman A. Barmin, MirJavad Moosavifar, Anshuman Dasgupta, Andreas Herrmann, Fabian Kiessling, Roger M. Pallares* and Twan Lammers*

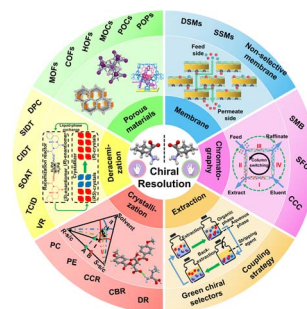


REVIEWS

11955

Strategies for chiral separation: from racemate to enantiomer

Jingchen Sui, Na Wang,* Jingkang Wang, Xin Huang, Ting Wang, Lina Zhou and Hongxun Hao*



Editorial Staff

Executive Editor

May Copsey

Deputy Editor

Samantha Apps

Senior Editor

James Moore

Scientific Editors

Ellis Crawford, Jingtao Huang, Esther Johnston, Sophie Orchard, Richard Thompson and Amy Welch

Editorial Assistant

Karina Webster

Publishing Assistant

David Bishop

For queries about submitted articles please contact James Moore, Senior Editor, in the first instance. E-mail chemicalscience@rsc.org

For pre-submission queries please contact May Copsey, Executive Editor. E-mail chemicalscience-rsc@rsc.org

Chemical Science (electronic: ISSN 2041-6539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

Chemical Science is a Gold Open Access journal and all articles from 2015 onwards are free to read.

Please email orders@rsc.org to register your interest or contact Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail orders@rsc.org

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

Chemical Science

rsc.li/chemical-science

Editorial Board

Editor-in-Chief

Andrew Cooper, University of Liverpool

Associate Editors

Vincent Artero, CEA-Grenoble
Luis M. Campos, Columbia University
Michelle Chang, University of California, Berkeley
Lin X. Chen, Northwestern University
Graeme Day, University of Southampton
Serena DeBeer, Max Planck Institute for Chemical Energy Conversion

Mircea Dincă, MIT

François Gabbai, Texas A&M University
Subi George, JNCASR
Ryan Gilmour, WWU Münster
Jinlong Gong, Tianjin University
Stephen Goldup, University of Birmingham
Zaiping Guo, University of Adelaide
Christopher A. Hunter, University of Cambridge
Malika Jefferies-EL, Boston University
Ning Jiao, Peking University
Tanja Junkers, Monash University

Hemamala Karunadasa, Stanford University
Maja Köhn, University of Freiburg
Yi-Tao Long, Nanjing University
Gabriel Merino, CINVESTAV Merida
James K. McCusker, Michigan State University
Thomas Meade, Northwestern University
Paolo Melchiorre, University of Bologna
Carsten Schultz, Oregon Health & Science University
Dmitri Talapin, The University of Chicago
Toshiharu Teranishi, Kyoto University
Andrei Yudin, University of Toronto

Advisory Board

D. Adams, University of Glasgow
A. Ajayaghosh, NIIST
R. Amaro, UC San Diego
A. Anastasaki, ETH Zürich
U.-P. Apfel, Ruhr-University Bochum
K. Asmis, Leipzig University
X. Bao, DICP-CAS
Z. Bao, Stanford University
D. N. Beratan, Duke University
G. Bernardes, University of Cambridge
F. Biedermann, KIT
D. Blackmond, Scripps Research Institute
E. Blasco, Heidelberg University
J. Bode, ETH Zurich
J. S. Brodbelt, UT Austin
C. Chang, UC Berkeley
C.-M. Che, University of Hong Kong
J. Chen, Nankai University
M. Cohen, OHSU
C. Coley, MIT
J. Cornella, MPIK
L. Cronin, University of Glasgow
J. Crowley, University of Otago
C. C. Cummins, MIT
V. Däschlein-Gessner, Ruhr University Bochum
M. Delbianco, MPICI
J. Dempsey, UNC Chapel Hill
W. Dichtel, Northwestern University
K. Domen, University of Tokyo
H. Duan, Tsinghua University
X. Feng, TU Dresden
B. Feringa, University of Groningen
J. Figueroa, UC San Diego
N. Frank, University of Nevada
M. Freitag, Newcastle University
S. Gao, Peking University
J. Gassensmith, UT Dallas
G. Gasser, PSL University
E. Gibson, Newcastle University
F. Glorius, WWU Münster
L. González, University of Vienna
D. Graham, University of Strathclyde
V. Grassian, UC San Diego
A. Grimaud, Collège de France/CNRS
T. Gulder, Leipzig University
W. Gutkunst, Georgia Tech
C. Hackenberger, FMP Berlin
I. Hamachi, Kyoto University
G. Han, Brandeis University
B. Han, CAS
M. Hariharan, IISER-TVM

C. Haynes, University of Minnesota
J. Heemstra, WUSTL
T. Heine, DTU
P. Holland, Yale University
K. E. Jelfs, Imperial College London
X. Jiang, Aramco
Y. Jung, SNU
S. Kath-Schorr, University of Cologne
T. Kato, University of Tokyo
C. Kelly, Janseen Research/J&J
R. Klausen, Johns Hopkins University
Y. Krishnan, University of Chicago
M. Kuimova, Imperial College London
K. Lancaster, Cornell University
A.-L. Lee, Heriot-Watt University
D. Leonori, University of Manchester
X. Li, University of Washington
Y. Li, Jilin University
M. H. Lim, KAIST
J. Lloret-Fillol, ICIQ
B. Lotsch, Max Planck Institute
X. W. Lou, NTU
K. Maeda, Tokyo Tech
S. Maeda, Hokkaido University
D. Maiti, IIT Bombay
L. Malins, ANU
S. Mandal, IISER Kolkata
T. Martinez, Stanford University
C. Martinez-Huitle, UFRN
E. Matson, Rochester University
J. L. Medina-Franco, UNAM
V. Moliner, INAM, Jaume I University
W. Nam, Ewha Womans University
T. Noël, University of Amsterdam
A. Obermeyer, Columbia University
M. Oestreich, TU Berlin
D. O'Hagan, University of St Andrews
T. Ooi, Nagoya University
R. O'Reilly, University of Birmingham
S. Ott, Uppsala University
H. Ottosson, Uppsala University
Z. Ouyang, Tsinghua University
X. Pan, DICP-CAS
S. Patil, SSCU-IISC
E. Pentzer, Texas A&M University
S. Peter, JNCASR
W. Piers, University of Calgary
N. Plumeré, Ruhr-University Bochum
S. Qiao, University of Adelaide
V. Rai, IISER Bhopal
S. Rasmussen, North Dakota State University

J. Read de Alaniz, UC Santa Barbara
E. Reisner, University of Cambridge
A. Rentmeister, WWU Munster
J. Rinehart, UC San Diego
A. Roitberg, University of Florida
H. Sardon, UPV-EHU
R. Sarpong, UC Berkeley
G. Schatz, Northwestern University
D. Schultz, Merck
D. Seferos, University of Toronto
R. Sessoli, University of Florence
H. Shafaat, UCLA
M. Kumova, Imperial College London
M. Solà, University of Girona
G. Soler-Illia, UNSAM
D. Spring, University of Cambridge
B. Sumerlin, University of Florida
R. B. Sunoj, IIT Bombay
Y. Surendranath, MIT
M. Tada, Nagoya University
T. Tahara, RIKEN
Z. Tang, NCNST
S. Teichert, DESY
C. Thomas, Ohio State University
H. Tian, ECUST
Z.-Q. Tian, Xiamen University
A. Tkatchenko, University of Luxembourg
H. Tran, University of Toronto
T. Uemura, University of Tokyo
C. Vanderwal, UC Irvine
L. Venkataraman, Columbia University
G. Vilé, Politecnico di Milano
A. Wakamiya, Kyoto University
L.-S. Wang, Brown University
C. Wang, Peking University
E. Weerapana, Boston College
J. Weinstein, University of Sheffield
T. Welton, Imperial College London
A. Wendlandt, MIT
C. Williams, University of Oxford
V. Yam, University of Hong Kong
N. Yanai, Kyushu University
S. Q. Yao, National University of Singapore
A. Zharbin, UFPR
L. Zhang, ECNU
T. Zhang, TIPC-CAS
J. Zhang, University of Cambridge
Z.-J. Zhao, Tianjin University
B. Zhong Tang, CUHK-Shenzhen
Q.-L. Zhou, Nankai University

Information for Authors

Full details on how to submit material for publication in Chemical Science are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/chemical-science

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered charity number: 207890

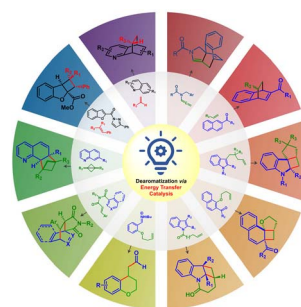


REVIEWS

12004

Rejuvenation of dearomative cycloaddition reactions via visible light energy transfer catalysis

Angshuman Palai, Pramod Rai and Biplab Maji*

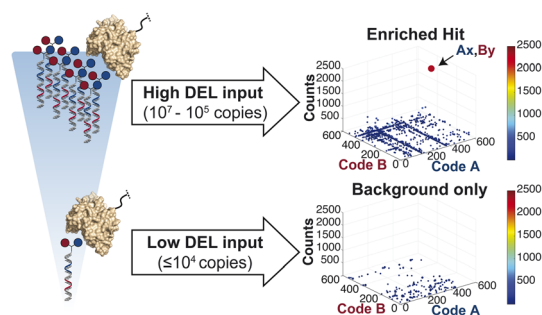


EDGE ARTICLES

12026

Impact of library input on the hit discovery rate in DNA-encoded chemical library selections

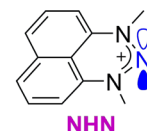
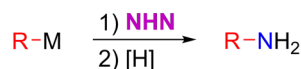
Sara Puglioli, Sebastian Oehler, Luca Prati, Jörg Scheuermann, Gabriele Bassi, Samuele Cazzamalli, Dario Neri* and Nicholas Favalli*



12034

Nitrenium ions as new versatile reagents for electrophilic amination

Idan Avigdori, Kuldeep Singh, Natalia Fridman and Mark Gandelman*

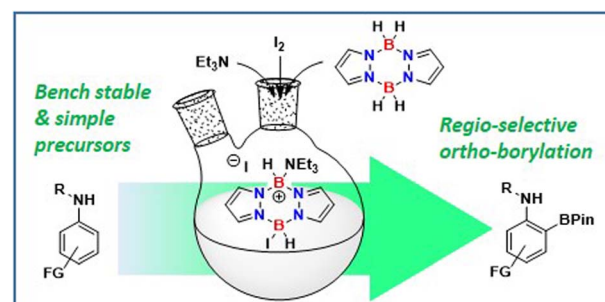


- ✓ *R* = 1°, 2°, 3° **alkyl** and diversely substituted **aryl** groups
- ✓ **Bench-stable**, non-oxidizing, easily prepared aminating agent
- ✓ One-pot synthesis of ¹⁵**N-labelled** biologically relevant amines
- ✓ Simple **recycling** procedure for the aminating agent

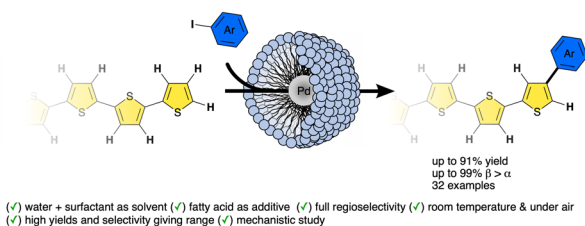
12041

Borylation directed borylation of *N*-alkyl anilines using iodine activated pyrazoboles

C. R. P. Millet, E. Noone, A. V. Schellbach, J. Pahl, J. Łosiewicz, G. S. Nichol and M. J. Ingleson*



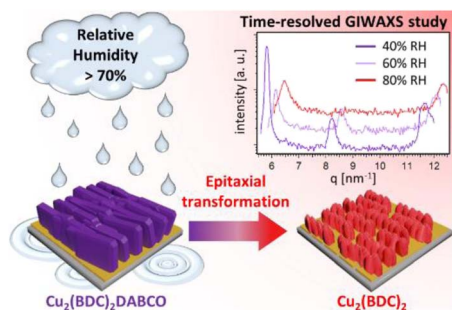
12049



Micellar catalysis: a green solution to enable undirected and mild C–H activation of (oligo) thiophenes at the challenging β -position

Pascal Hauk, Valérie Mazan, Fabrice Gallou* and Joanna Wencel-Delord*

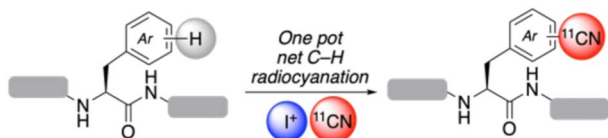
12056



Water sensitivity of heteroepitaxial Cu-MOF films: dissolution and re-crystallization of 3D-oriented MOF superstructures

Lea A. Brandner, Mercedes Linares-Moreau, Guojun Zhou, Heinz Amenitsch, Simone Dal Zilio, Zhehao Huang, Christian Doonan* and Paolo Falcaro*

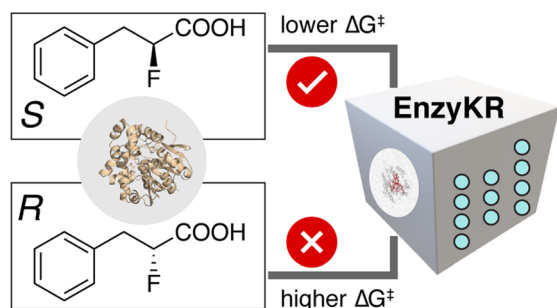
12068



C–H radiocyanation of bioactive molecules *via* sequential iodination/copper-mediated cross-coupling

Mami Horikawa, Stephen T. Joy, Liam S. Sharninghausen, Xia Shao, Anna K. Mapp,* Peter J. H. Scott* and Melanie S. Sanford*

12073



EnzyKR: a chirality-aware deep learning model for predicting the outcomes of the hydrolase-catalyzed kinetic resolution

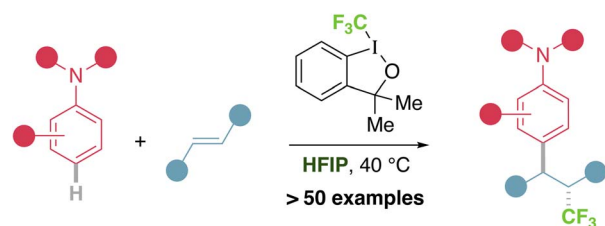
Xinchun Ran, Yaoyukun Jiang, Qianzhen Shao and Zhongyue J. Yang*



12083

Trifluoromethylarylation of alkenes using anilines

Carlos Corral Suarez and Ignacio Colomer*

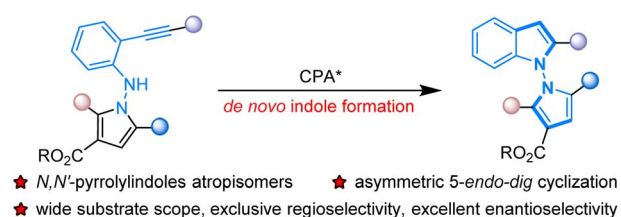


- ✓ metal- and photocatalyst-free
- ✓ chemo- regio- and stereocontrol
- ✓ mechanistic studies
- ✓ drug functionalization

12091

Organocatalytic atroposelective synthesis of axially chiral *N,N'*-pyrrolylindoles via *de novo* indole formation

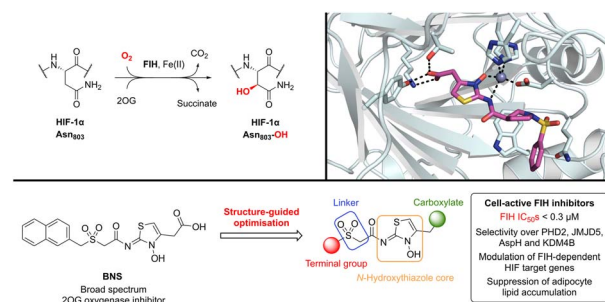
Cong-Shuai Wang, Qi Xiong, Hui Xu, Hao-Ran Yang, Yanfeng Dang,* Xiu-Qin Dong* and Chun-Jiang Wang*



12098

Structure-guided optimisation of *N*-hydroxythiazole-derived inhibitors of factor inhibiting hypoxia-inducible factor- α

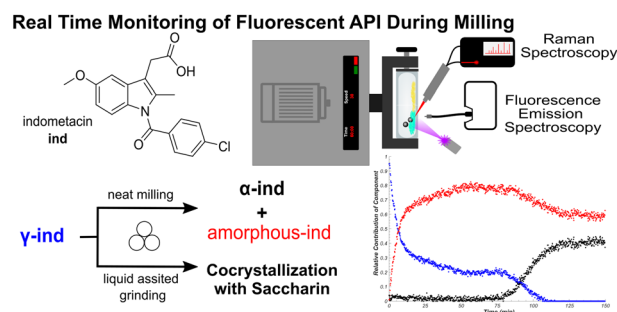
Thomas P. Corner, Ryan Z. R. Teo, Yue Wu, Eidarus Salah, Yu Nakashima, Giorgia Fiorini, Anthony Tumber, Amelia Brasnett, James P. Holt-Martyn, William D. Figg, Jr., Xiaojin Zhang,* Lennart Brewitz* and Christopher J. Schofield*



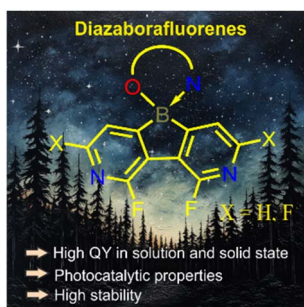
12121

Illuminating milling mechanochemistry by tandem real-time fluorescence emission and Raman spectroscopy monitoring

Patrick A. Julien,* Mihails Arhangelskis,* Luzia S. Germann, Martin Etter, Robert E. Dinnebier, Andrew J. Morris* and Tomislav Friščić*



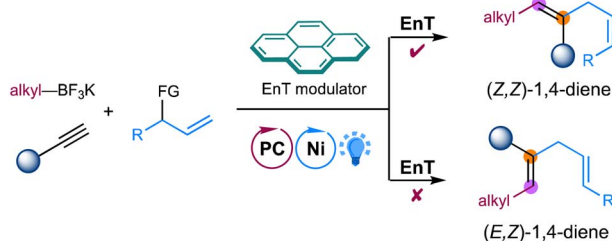
12133



Highly electron-deficient 3,6-diaza-9-borafluorene scaffolds for the construction of luminescent chelate complexes

Jan Adamek, Paulina H. Marek-Urban, Krzysztof Woźniak, Krzysztof Durka* and Sergiusz Luliński*

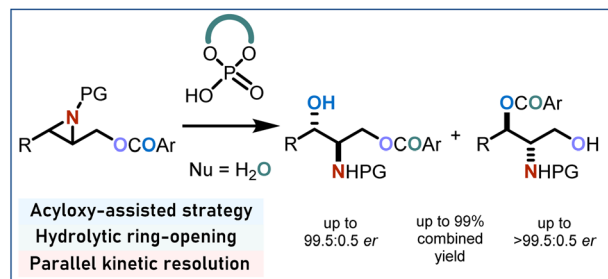
12143



Divergent 1,2-carboallylation of terminal alkynes enabled by metallaphotoredox catalysis with switchable triplet energy transfer

Jian Qin, Zhuzhu Zhang, Yi Lu, Shengqing Zhu and Lingling Chu*

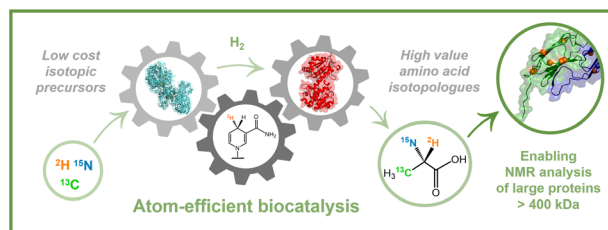
12152



Parallel kinetic resolution of aziridines via chiral phosphoric acid-catalyzed apparent hydrolytic ring-opening

Juan Liu, Yi-Ying Du, Yu-Shi He, Yan Liang, Shang-Zhong Liu, Yi-Yi Li and Yi-Ming Cao*

12160



Biocatalytic reductive amination as a route to isotopically labelled amino acids suitable for analysis of large proteins by NMR

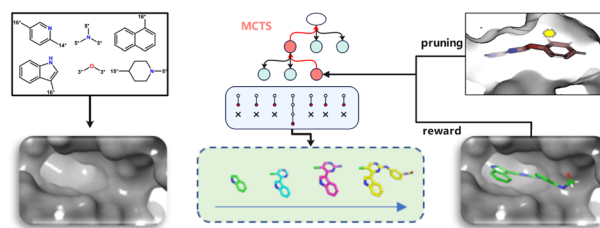
Jack S. Rowbotham,* Jake H. Nicholson, Miguel A. Ramirez, Kouji Urata, Peter M. T. Todd, Gogulan Karunanithy, Lars Lauterbach, Holly A. Reeve, Andrew J. Baldwin* and Kylie A. Vincent*



12166

A flexible data-free framework for structure-based *de novo* drug design with reinforcement learning

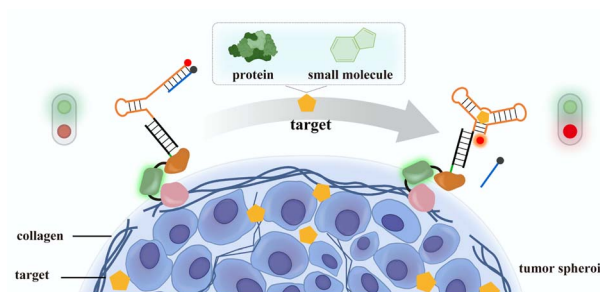
Hongyan Du, Dejun Jiang, Odin Zhang, Zhenxing Wu, Junbo Gao, Xujun Zhang, Xiaorui Wang, Yafeng Deng, Yu Kang, Dan Li, Peichen Pan,* Chang-Yu Hsieh* and Tingjun Hou*



12182

A collagen-immobilized nanodevice for *in situ* ratiometric imaging of cancer biomarkers in the tumor microenvironment

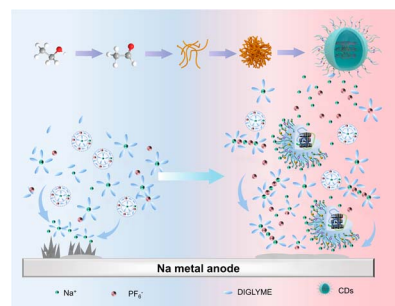
Fengyu Tian, Shurui Zhou, Shiyi Xie, Zhenhua Zhang, Ling Peng, Ling Jiang, Zeyuan Wang, Zhou Nie and Yan Huang*



12194

Carbon dots from alcohol molecules: principles and the reaction mechanism

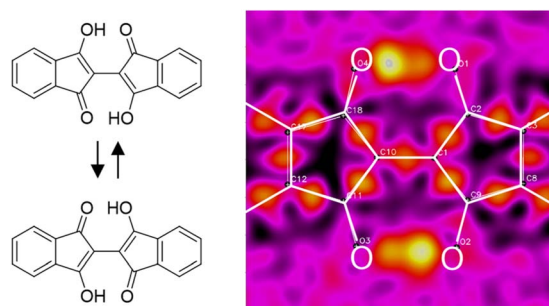
Hanyu Tu, Huaxin Liu, Laiqiang Xu, Zheng Luo, Lin Li, Ye Tian, Wentao Deng, Guoqiang Zou, Hongshuai Hou* and Xiaobo Ji*



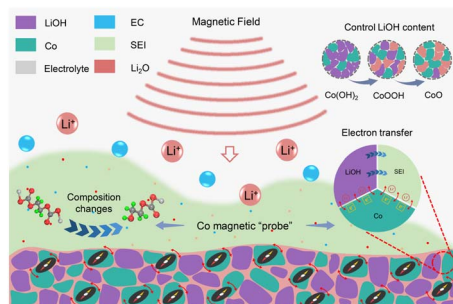
12205

Synthesis of 3,3'-dihydroxy-2,2'-diindan-1,1'-dione derivatives for tautomeric organic semiconductors exhibiting intramolecular double proton transfer

Kyohei Nakano, Iat Wai Leong, Daisuke Hashizume, Kirill Bulgarevich, Kazuo Takimiya, Yusuke Nishiyama, Toshio Yamazaki and Keisuke Tajima*



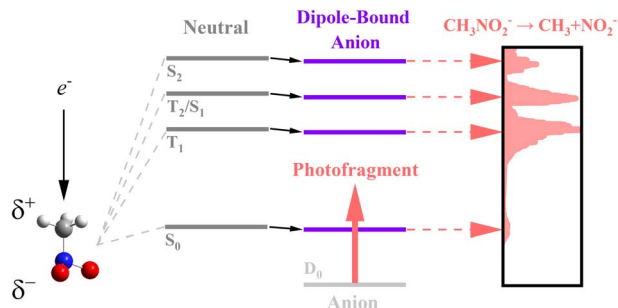
12219



Revealing the effect of LiOH on forming a SEI using a Co magnetic "probe"

Zhiqiang Zhao, Wanneng Ye, Fengling Zhang, Yuanyuan Pan, Zengqing Zhuo, Feihu Zou, Xixiang Xu, Xiancheng Sang, Weiqi Song, Yue Zhao, Hongsen Li, Kuikui Wang, Chunfu Lin, Han Hu,* Qinghao Li,* Wanli Yang and Qiang Li*

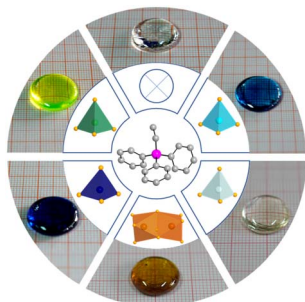
12231



Excited-state chemistry of the nitromethane anion mediated by the dipole-bound states revealed by photofragment action spectroscopy

Sejun An, Dabin Kim, Junggil Kim and Sang Kyu Kim*

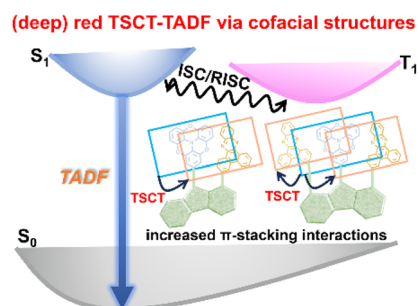
12238



In situ recrystallization of zero-dimensional hybrid metal halide glass-ceramics toward improved scintillation performance

Bohan Li, Jiance Jin, Meijuan Yin, Kai Han, Yuchi Zhang, Xinlei Zhang, Anran Zhang, Zhiguo Xia* and Yan Xu*

12246



Simultaneously enhancing the planarity and electron-donating capability of donors for through-space charge transfer TADF towards deep-red emission

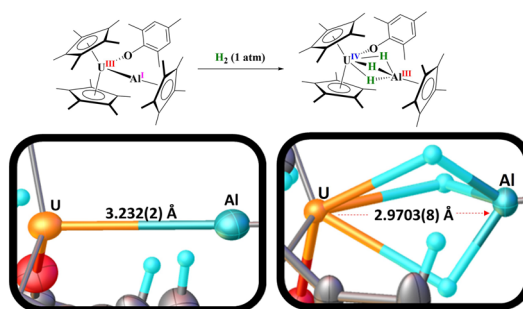
Xiu-Fang Song, Chenglin Jiang, Nengquan Li, Jingsheng Miao, Kai Li* and Chuluo Yang*



12255

Cooperative dihydrogen activation with unsupported uranium–metal bonds and characterization of a terminal U(IV) hydride

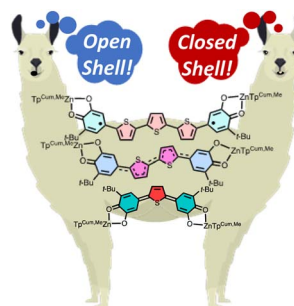
Robert J. Ward, Pokpong Rungthanaphatsophon, Patrick Huang, Steven P. Kelley and Justin R. Walensky*



12264

Variation from closed-shell to open shell electronic structures in oligothiophene bis(dioxolene) complexes

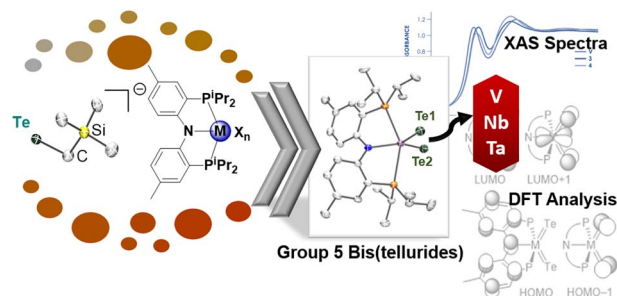
Paul D. Miller, David A. Shultz,* Joshua Mengell, Martin L. Kirk* and Lukasz Wojtas



12277

Tellurolate: an effective Te-atom transfer reagent to prepare the triad of group 5 metal bis(tellurides)

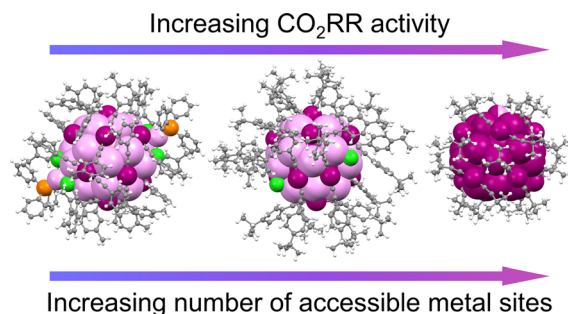
Shuruthi Senthil, Seongyeon Kwon, Richard Y. Kong, Samantha N. MacMillan, Pavel Zatsepin, Michael R. Gau, Patrick J. Carroll, Mu-Hyun Baik,* Kyle M. Lancaster* and Daniel J. Mindiola*



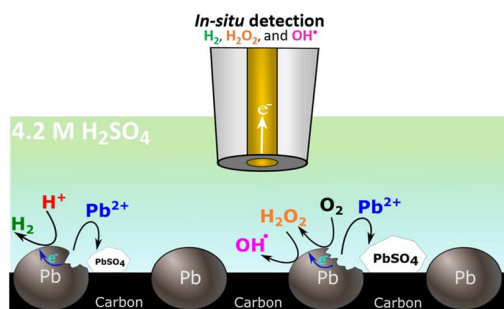
12283

The role of metal accessibility on carbon dioxide electroreduction in atomically precise nanoclusters

Yingwei Li, Grant J. Stec, Agnes E. Thorarinsdottir, Ryan D. McGillicuddy, Shao-Liang Zheng and Jarad A. Mason*



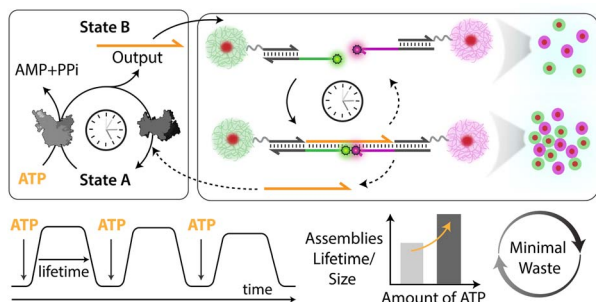
12292



In situ detection of reactive oxygen species spontaneously generated on lead acid battery anodes: a pathway for degradation and self-discharge at open circuit

Abdelilah Asserghine, Aravind Baby, Seth T. Putnam, Peisen Qian, Elizabeth Gao, Huimin Zhao and Joaquín Rodríguez-López*

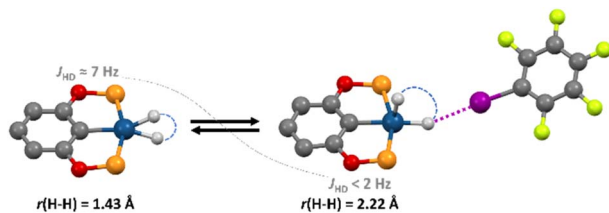
12299



Transient co-assemblies of micron-scale colloids regulated by ATP-fueled reaction networks

Charu Sharma, Aritra Sarkar and Andreas Walther*

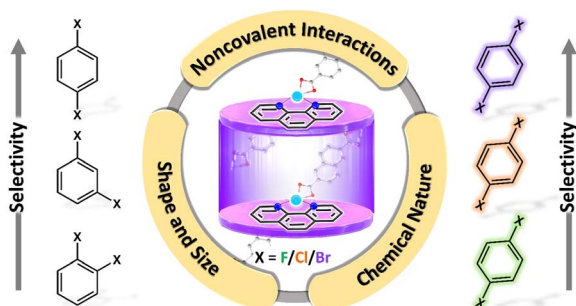
12308



Unravelling strong temperature-dependence of J_{HD} in transition metal hydrides: solvation and non-covalent interactions *versus* temperature-elastic H-H bonds

Alexey V. Polukeev,* Silvia C. Capelli and Ola F. Wendt

12321



Noncovalent interaction guided selectivity of haloaromatic isomers in a flexible porous coordination polymer

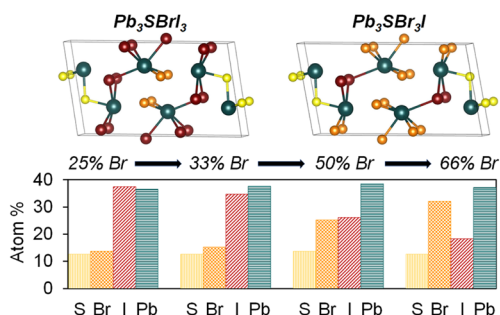
Rohan Jena, Subhajit Laha, Nimish Dwarkanath, Arpan Hazra, Ritesh Halder,* Sundaram Balasubramanian* and Tapas Kumar Maji*



12331

Designing complex $Pb_3SBr_xI_{4-x}$ chalcogenides: tunable emission semiconductors through halide-mixing

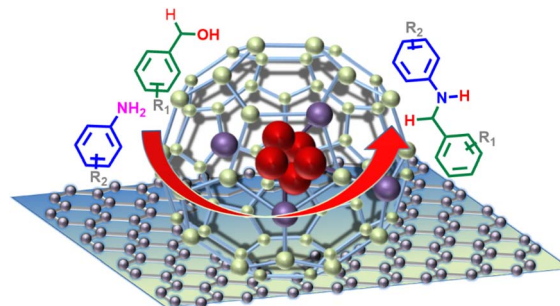
Alison N. Roth, Yunhua Chen, Anuluxan Santhiran, Jemima Opare-Addo, Eunbyeol Gi, Emily A. Smith, Aaron J. Rossini and Javier Vela*



12339

Metal-organic framework-derived CoN_x nanoparticles on N-doped carbon for selective *N*-alkylation of aniline

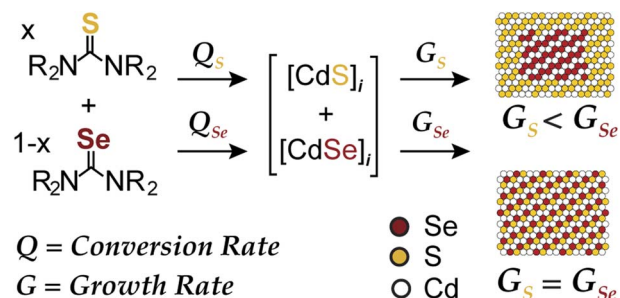
Ved Vyas, Priyanka Maurya and Arindam Indra*



12345

Synthesis of graded $CdS_{1-x}Se_x$ nanoplatelet alloys and heterostructures from pairs of chalcogenoureas with tailored conversion reactivity

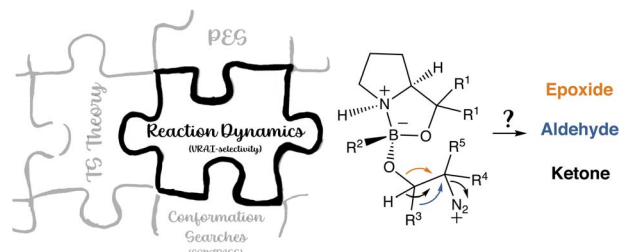
Natalie Saenz, Leslie S. Hamachi, Anna Wolock, Berit H. Goodge, Alexis Kuntzmann, Benoit Dubertret, Isabel Billinge, Lena F. Kourkoutis, David A. Muller, Andrew C. Crowther and Jonathan S. Owen*



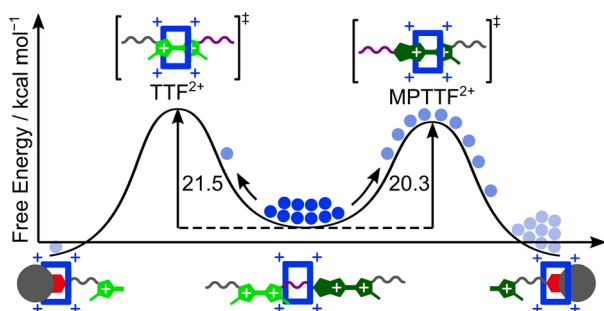
12355

Reaction dynamics as the missing puzzle piece: the origin of selectivity in oxazaborolidinium ion-catalysed reactions

Ching Ching Lam and Jonathan M. Goodman



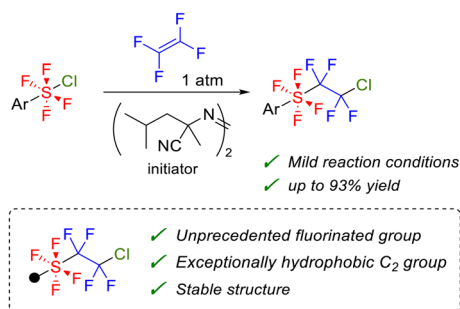
12366



Mechanistic studies of isomeric [2]rotaxanes consisting of two different tetrathiafulvalene units reveal that the movement of cyclobis(paraquat-*p*-phenylene) can be controlled

Sofie K. Jensen, Mathias S. Neumann, Rikke Frederiksen, Mathias L. Skavenborg, Mads C. Larsen, Stinne E. Wessel and Jan O. Jeppesen*

12379



Fluoroalkylated hypervalent sulfur fluorides: radical addition of arylchlorotetrafluoro-λ⁶-sulfanes to tetrafluoroethylene

Eisuke Yasuo, Kohsuke Aikawa,* Kyoko Nozaki and Takashi Okazoe

CORRECTION

12386

Correction: Structurally divergent enantioselective synthesis of benzofuran fused azocine derivatives and spiro-cyclopentanone benzofurans enabled by sequential catalysis

Rupkumar Khuntia, Sanat Kumar Mahapatra, Lisa Roy and Subhas Chandra Pan*

